Direct Simulation Monte Carlo: Theory, Methods, and Open Challenges

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ABSTRACT

These lecture notes present the basic theory and methods for the Direct Simulation Monte Carlo (DSMC) algorithm. Some of the open challenges in the treatment of complex, multi-scale flows are also discussed.

1.0 INTRODUCTION

1.1 Dynamics of Dilute Gases

Figure 1 illustrates the large range of physical scales for dilute gases, ranging from the quantum scale to the hydrodynamic scale. At the smallest scales, the details of the intermolecular interaction are important; the corresponding time scale is the duration time of a collision, which is on the order of femtoseconds. At the opposite end, when the gas is well-represented by continuum hydrodynamic fields (density, temperature, etc.) then a description based on partial differential equations, such as the Navier-Stokes equations, is accurate.

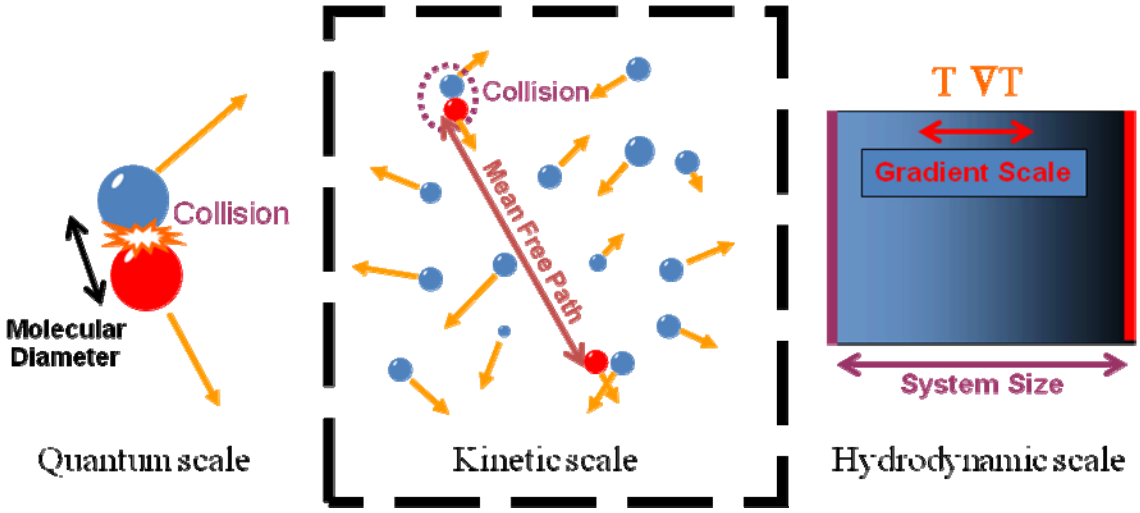

Figure 1: Physical scales for dilute gases.

At the intermediate, kinetic scale the discrete molecular nature of the gas has a significant effect on the dynamics. The relevant length and time scales in this regime are the mean free path and mean free time and they establish all the transport properties. At this scale the continuum approximations for transport, such as the Fourier law for heat flux, are not accurate so standard Computational Fluid Dynamics (CFD) approaches are not suitable. On the other hand, the collisions themselves may accurately be treated using a simplified classical approximation or as stochastic events with specified rates.

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1.2 Direct Simulation Monte Carlo

Direct Simulation Monte Carlo (DSMC) is a molecular scheme designed for the simulation of gases at the kinetic scale. [1] DSMC was developed by Graeme Bird in the late 1960's for kinetic scale simulations and was quickly adopted by the aerospace engineering community because the method is accurate for flows with high Knudsen number (Kn), the ratio of mean free path to system length. For example, during the initial re-entry flight in the upper atmosphere the mean free path in the air is comparable to the size of the vehicle. Although DSMC was originally motivated by these "Space Age" applications, the method is now used in a wide range of problems in physics, chemistry, and engineering. Examples range from micron-scale flows (which are also high Knudsen number) to granular gases to lunar atmospheres. The algorithm has evolved as well, with improvements to the numerical accuracy and efficiency as well as extensions to complex chemistry and even to dense gases. Nearly 50 years after its introduction DSMC remains the dominant numerical method for molecular simulations of dilute gases.

1.3 Molecular Dynamics and DSMC

Molecular Dynamics (MD) is another popular numerical approach for molecular simulations but it is normally applied to liquids. [2] In MD the exact molecular motion is calculated from the inter-molecular forces among the particles. Although this may be done efficiently for liquids, in which the molecules directly interact with only a few neighbouring molecules, in a dilute gas a molecule has thousands of potential collision partners. Direct Simulation Monte Carlo (DSMC) overcomes the inefficiency of MD by replacing the deterministic motion with a stochastic approximation for the collision process. DSMC is able to advance in time steps comparable to the mean free time between collisions yet remain accurate at the level of the Boltzmann equation. Unlike MD, DSMC is always numerically stable regardless of time step.

2.0 DSMC METHOD

2.1 Outline of DSMC

Before describing the details of how DSMC works, let us quickly outline the algorithm's framework. DSMC is a particle-based scheme so a typical calculation initializes the desired geometry with boundary conditions and fills the computational volume with random particles. At each time step all particles move ballistically according to their assigned velocity; in DSMC collisions are *independent* of these trajectories. Any particles reaching a boundary are processed according to the imposed conditions, such as randomly assigning a new velocity to a particle that strikes a thermal wall. If there are open boundaries (e.g., wind-tunnel configuration) then particles are generated as inflow and removed if they exit through the boundary. Quantities of interest in a simulation are either flow properties (e.g., temperature field in the flow) or surface quantities (e.g., drag and lift for a vehicle) and these are measured by statistical samples of particles contained in a volume or striking a surface. Finally, DSMC randomly selects and evaluates collisions among the particles. This last step is the heart of the algorithm so it will be described in some detail.

2.2 Random Numbers

As its name implies, Direct Simulation Monte Carlo uses random numbers. Unlike other Monte Carlo schemes, such as Metropolis MC or Quantum MC, DSMC uses a wide variety of probability distributions for different purposes. For example, to initialize particles in a volume we might first determine the number of particles to insert by choosing the value from a Poisson distribution. If the particles are distributed uniformly then their coordinates are generated from the uniform distribution; their velocity components are usually generated from the Maxwell-Boltzmann distribution, which is equivalent to a normal or Guassian distribution. As described below, at various stages of the advection and collision processes more random variables are used from various distributions.

Given the importance of the Monte Carlo elements in DSMC it is essential to use a high-quality random number generator. Simple generators that were adequate a decade ago are obsolete today because, with increased computer power, modern DSMC calculations can cycle through the entire period of a simple generator in a matter of seconds. Although DSMC generates random values from a variety of distributions, the program only needs one generator that produces the uniform distribution in (0,1); all other distributions are obtained by transformation (usually inversion of the cumulative distribution) or iteration (typically an acceptance / rejection scheme). [3] There are several modern generators for the uniform distribution to choose from; the author's current favourite is the Mersenne Twister. [4] One final note regarding the use of random number generators: for the purpose of debugging the initial state (or seed) should be recorded so that a calculation that fails can be repeated exactly.

2.3 Boundary Conditions

Once the particles have been initialized the DSMC calculation advances in time steps Δt, alternating between ballistic motion of the particles and collisions among the particles. Typically the particles simply are displaced by a distance $\Delta \boldsymbol{r} = \boldsymbol{v}\,\Delta t$ but if there is a body force, such as gravity, then the motion is slightly more complicated. The particles move without interaction and can even overlap; the only place in DSMC where the particles' cross-section is used is in determining the collision rate. For transient flows, on the first time step one should use ½ Δt (Strang splitting) to maintain temporal accuracy. If measuring non-conserved variables (e.g., fluxes) then one should also time-center the sampling (half move, sample, half move, collisions) for all steps.

During their motion some of the particles will reach boundaries, either at the periphery of the computational domain or at the surfaces of objects within the domain. One of the strengths of DSMC is the ease with which boundary conditions may be imposed. For periodic boundaries a particle crosses one boundary and re-enters at the periodic mirror boundary. For specular boundaries a particle reflects off the surface with the perpendicular component of velocity reversed. At a thermal wall a particle's velocity components are reset according to the biased-Maxwellian distribution for the normal component

$$P_\perp(v_\perp) = \frac{m}{kT_w} v_\perp e^{-mv_\perp^2/2kT_w}$$

and the standard Maxwell-Boltzmann distribution for the parallel components,

$$P_\parallel(v_\parallel) = \sqrt{\frac{m}{2\pi kT_w}}, e^{-mv_\parallel^2/2kT_w}$$

Both of these distributions are easily generated by inversion, the former from an exponential distribution and the latter from a normal distribution. A surface may not be fully accommodating, for example in the Maxwell model a random fraction, α, are thermalized while the rest reflect specularly.

Inflow/outflow boundary conditions are commonly treated as a reservoir with given density, fluid velocity, temperature. Particles in the main system are removed if they cross the boundary into the reservoir. Particles are injected from reservoir to main system by either: *Surface generator* - From the number flux determine number to be injected during a time step and then generate particle velocities from surface distribution (e.g., inflow Maxwellian); *Volume generator* - Fill a "ghost cell" with particles before the ballistic move and discard any that do not cross the boundary into the main system during the move phase. Efficient schemes are available for both types of generators. [5,6]

2.4 Collision Selection

To evaluate collisions the domain is partitioned into cells and the particles are sorted into them; the algorithm then loops over cells evaluating collisions independently in each cell. A maximum collision rate, $R_{max} = R(N, V, \sigma, \max\{v_r\})$, is calculated in each cell based on the number of particles, the cell volume, the collisional cross-section for the particles, and the (estimated) maximum relative speed. The explicit form for this function depends on the interaction potential; for example, for hard spheres,

$$R(N, V, \sigma, v_r) = \frac{N(N-1)\sigma v_r}{2V}$$

where $\sigma = \pi d^2$. The mean collision rate is

$$\langle R \rangle = \frac{\langle N \rangle^2 \sigma \langle v_r \rangle}{2V}$$

since N is Poisson distributed. The number of attempted collisions during a time step is $R_{max}\,\Delta t$; for each attempted collision a random pair of particles is selected within the cell. Given the actual relative velocity for the selected pair, they are accepted as collision partners with probability $R(N, V, \sigma, v_r)/R_{max}$. This not only accepts pairs with the correct probability (pairs with higher relative velocity are more likely to collide) but also accepts them with the correct mean collision rate.

2.5 Collision Evaluation

Once a pair is accepted for a collision all that remains is the calculation of the particles' post-collision velocities (if there are also internal degrees of freedom or chemistry then there are addition steps). By conservation of momentum the center-of-mass velocity is constant; for particles of equal mass, conservation of energy implies that the magnitude of the relative velocity is unchanged. These constraints fix four of the six unknowns; the remaining two are set by the direction angle for the relative velocity. Because DSMC does not use the actual particle trajectories to evaluate collisions this direction angle is selected at random. For hard-sphere collisions the direction angle is chosen as uniformly distributed in the unit sphere by inversion. [3]

2.6 DSMC "Parliament"

In DSMC the number of simulation particles ("simulators") is typically a small fraction of the number of physical molecules with each simulator representing N_{ef} physical molecules. DSMC's dynamics is correct if: a) The DSMC simulators are an unbiased sample of the physical population (unbiased parliament); b) Collision rate is increased by N_{ef} so the number of collisions per unit time for a simulator is same as for a physical molecule; c) In sampling, each simulator counts as N_{ef} physical molecules. Early DSMC implementations used a different (unpopular) representation, rescaling the simulator diameter and mass to maintain the same physical mean free path and mass density. While increasing N_{ef} and lowering the number of simulators speeds the calculation it also decreases the accuracy. Empirically it has been found that the accuracy of DSMC goes as $1/N$; for traditional DSMC keeping about N=20 particles per collision cell is the rule-of-thumb. [7]

2.7 Ballistic and Collisional Transport

By their ballistic motion particles carry mass, momentum and energy. In a dilute gas, this is the *only* physical mechanism for transport. Yet in DSMC, momentum and energy are also transported by the collisions. The larger the collision cell, the more collisional transport because of the greater average separation between particle pairs. The collisional transport may be calculated by Green-Kubo theory,

which finds that this error is quadratic in cell size and time step. [8,9] To minimize this collisional transport the rule-of-thumb for traditional DSMC is to limit the cell size to a fraction of a mean free path and the time step to a fraction of a mean collision time. New DSMC implementations minimize collisional transport error by choosing the collision partner as the nearest particle in the cell. To avoid bias due to re-collisions, a particle pair is not allowed to collide twice (choose next-nearest particle instead). Two common implementations are: Transient Adaptive Sub-cells (introduced by Bird); and Virtual Sub-cells (introduced by LeBeau, et al). [10]

3.0 HYDRODYNAMIC FLUCTUATIONS AND STATISTICAL ERROR

3.1 Fluctuations in DSMC

Even at thermodynamic equilibrium, the state of the system in DSMC has random variations as particles move and collide. It is important to note that these hydrodynamic fluctuations in density, temperature, etc. have *nothing* to do with the Monte Carlo aspect of DSMC. Molecular Dynamics is a deterministic algorithm and it has precisely the same fluctuations. The random variations in particle-based schemes arise from the complex ergotic mixing dynamics due to the non-linear interactions.

The variance of fluctuations in DSMC is exact at equilibrium; particles are uniformly distributed in position and their velocities are Maxwell-Boltzmann distributed. The spatial and temporal correlations of fluctuations in DSMC are also correct at hydrodynamic scales, as demonstrated by the agreement found with Landau-Lifshitz fluctuating hydrodynamics, and beyond. [11] Surprisingly, this agreement extends to strongly non-equilibrium scenarios such as severe temperature gradients and strong shearing flows. [12]

If the phenomenon of interest has dynamics that depend on the accurate representation of fluctuations, such as Brownian motion, then the fluctuations in DSMC are a positive feature. However, for most engineering applications these fluctuations are an annoyance because of the amount of sampling that has to be done in order to extract accurate answers. Furthermore, when each DSMC simulation particle represents a large number of physical molecules, as is typical in engineering calculations, the variance of fluctuations is magnified by this ratio. For this reason fluctuations are unphysically large when $N_{ef} > 1$.

3.2 Error Bars in DSMC

Fortunately, because the variances of fluctuations in DSMC are known from statistical mechanics, we may estimate *a priori* the amount of sampling needed to obtain the desired accuracy. Furthermore, since the non-equilibrium corrections are small, even when gradients are large, we may use the simpler results for equilibrium fluctuations for estimating error bars. [13] For example, the fractional error in the sample mean of the *x*-component of fluid velocity is

$$E_u = \frac{\sigma_u}{|u_x|} = \frac{\sqrt{\langle \delta u_x^2 \rangle}/\sqrt{S}}{|u_x|} \approx \frac{1}{\sqrt{SN}} \frac{1}{\mathrm{Ma}}$$

where S is the number of samples, N is the average number of DSMC particles in the sampling volume, and Ma is the Mach number of the flow. We immediately see that in aerospace applications, where the Mach number is large, only a small number of samples is required. In microscopic flows, where Ma << 1, the fractional error is much greater and far more sampling is required, especially since the error bar magnitude decreases as $S^{-1/2}$. Similar results are found for other hydrodynamic quantities and these results apply equally to other particle-based schemes, such as Molecular Dynamics.

3.3 Variance Reduction

Attempts to reduce the variance in DSMC have had mixed success. Some approaches are effective but at the expense of introducing significant complexity to the calculations of collisions, advection, boundary conditions, etc. Other approaches are simple to implement but are not always numerically stable. Worst of all are those approaches that inadvertently introduce statistical errors that bias the sampling. For example, if the cells into which particles are partitioned are dynamically resized (for example, to use larger cell volumes in regions with few simulation particles) then the cell volume is a random variable, possibly correlated to other variables. In general $\langle 1/V \rangle \neq 1/\langle V \rangle$ so calculations involving density (e.g., collision rate) will have a statistical bias depending on the probability distribution for volume. Nevertheless, there has recently been promising progress in variance reduction for DSMC (and its variants) and this remains an active and important topic for research. [14, 15]

3.1 Thermal Fluctuations and Brownian Dynamics

Returning to the positive viewpoint of fluctuations, there are a number of important applications where the stochastic nature of a fluid at microscopic scales is central to the phenomenon of interest. The accurate modelling of multi-scale fluid phenomena often requires the correct representation of the spatial and temporal spectra of fluctuations, specifically when studying systems where the microscopic stochastics drive macroscopic phenomena. Some examples in which spontaneous fluctuations play an important role in hydrodynamics include the breakup of droplets in jets, Rayleigh-Bernard convection, Kolmogorov flow, and Rayleigh-Taylor mixing. Thermal fluctuations are also important in many chemical phenomena, such as combustion and explosive detonation as well as the propagation of reaction fronts. Finally, micro-machines have been proposed that make use of spontaneous fluctuations as an essential part of the design. In fact many biological mechanism operating at the cellular level employ such “Brownian motors.” In *Directing Matter and Energy: Five Challenges for Science and the Imagination*, a report by the Basic Energy Sciences Advisory Committee, the authors state that, ``evolution has embraced stochastic fluctuations and often relies on them for the functionality of the system. This suggests an interesting design principle that humans have not yet learned to use. Exploitation of statistical fluctuations may well be essential to accomplish some of the more exotic tasks living systems are able to perform...Realizing the promise of nanoscience requires that we deal with non-equilibrium and fluctuations." Because DSMC simulations include spontaneous fluctuations with the correct physical spectrum (when $N_{ef} = 1$) the method is ideally suited for these types of problems in dilute gases.

4.0 ALGORITHM REFINEMENT

4.1 Multi-Scale Modeling

Algorithm Refinement (AR) is an important new approach for modeling multiscale fluid phenomena. Based on the framework of mesh refinement, AR combines two or more algorithms that use different descriptions of the flow at different scales. Such hybrid schemes typically couple structurally different computational schemes such as particle-based molecular simulations with continuum partial differential equation (PDE) solvers. The general idea is to perform detailed calculations using an accurate but expensive algorithm in a small region (or for a short time), and couple this computation to a simpler, less expensive method applied elsewhere.

Algorithm Refinement addresses several difficulties associated with multi-scale numerical modelling. First, the wide range of salient scales makes it impractical or impossible, even with the next generation of supercomputers, to perform full system calculations using algorithms that capture the correct physics at the finest resolution. Second, numerical approaches that rely on continuum models and constitutive closure relations are limited by the underlying assumptions (which are often phenomenological and sometimes not well understood), leading to erroneous predictions if used in regimes where these

approximations break down. Finally, mathematical models use disparately different representations for molecular, mesoscopic, or macroscopic scales, and the corresponding algorithms echo this disparity. Although the mathematical models and corresponding numerical methodologies used in hybrid schemes are often mature techniques, problems can arise because the various methods are usually developed independently with little consideration to their coupling to other models or methods appropriate for other scales. Naive attempts to reduce the computational expense of molecular simulations by combining them with simple continuum models have often resulted in ad-hoc constructions that are numerically inaccurate, unstable, and inefficient because the two algorithms were simply cobbled together.

4.2 Algorithm Refinement with DSMC

The coupling of DSMC with a continuum CFD solver was introduced over 20 years ago [16] and many implementations have been presented in the literature. Most of these hybrids have been aerospace engineering codes; as described in the previous section, spontaneous fluctuations in DSMC are an annoyance for those applications. On the other hand, the group at Lawrence Berkeley lab has been developing DSMC/CFD hybrids with an eye towards complex, stochastic flows. Figure 2 schematically illustrates the formulation of an AR hybrid for the Brownian motion of a sphere.

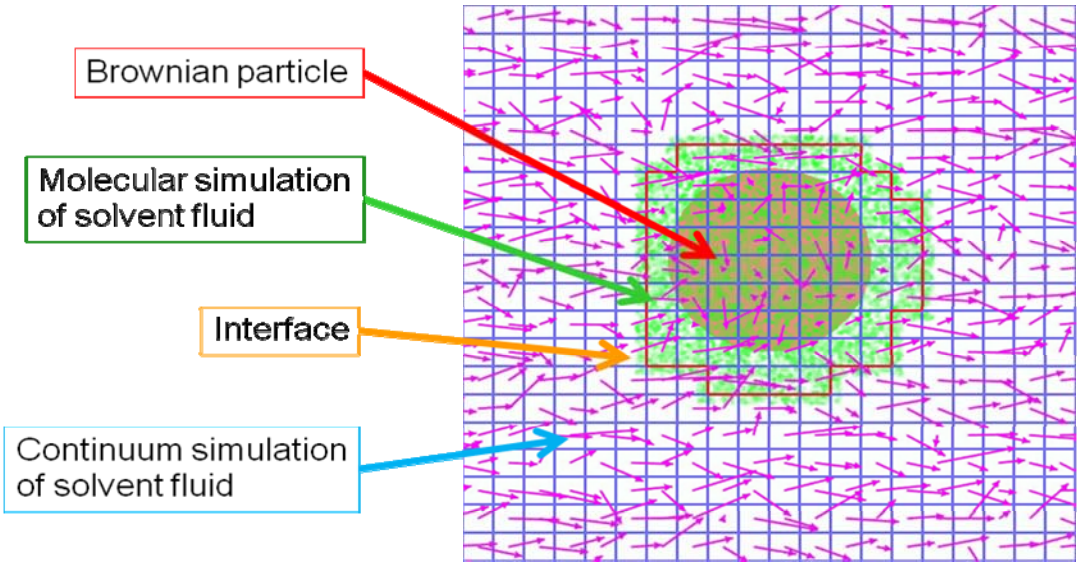

Figure 2: Algorithm Refinement hybrid coupling a DSMC calculation near the Brownian particle and a continuum PDE calculation in the bulk of the fluid.

Our research has been directed along three avenues: First, our original AR scheme [17] was limited to dilute gases using DSMC but we have developed more advanced stochastic particle schemes for non-ideal fluids. These are discussed in Section 5. Second, perfecting the coupling of particle and PDE schemes is challenging due to fluctuations. Though our coupling is still not entirely seamless, we have a better understanding as to the physical origin of the mismatch. Finally, in the past we used a deterministic, explicit scheme for the full Navier-Stokes equations but we now have efficient, accurate stochastic PDE schemes for the Landau-Lifshitz fluctuating hydrodynamic equations.[18,19]

4.3 Hybrids with Stochastic PDE Solvers

While a stochastic PDE solver is not difficult to implement, the question naturally arises: Is it necessary to include accurate hydrodynamic fluctuations in the continuum region given that the particle region, which surrounds the Brownian particle, already has fluctuations? The answer is a resounding yes, as we

discovered in two basic examples. [20] First, the velocity auto-correlation function for the Brownian particle is accurately reproduced by an AR hybrid with stochastic PDEs but not with deterministic PDEs. The second example is the "adiabatic piston", illustrated in Figure 3. Molecules collide specularly with the massive piston, which then performs an asymmetric Brownian walk until the gases on the two sides reach mechanical and thermal equilibrium (i.e., equal pressure and temperature). In Figure 4 we clearly see that the equilibration of the piston position with time is incorrect for the deterministic hybrid, even though the particle region is centred adaptively to follow the piston position.

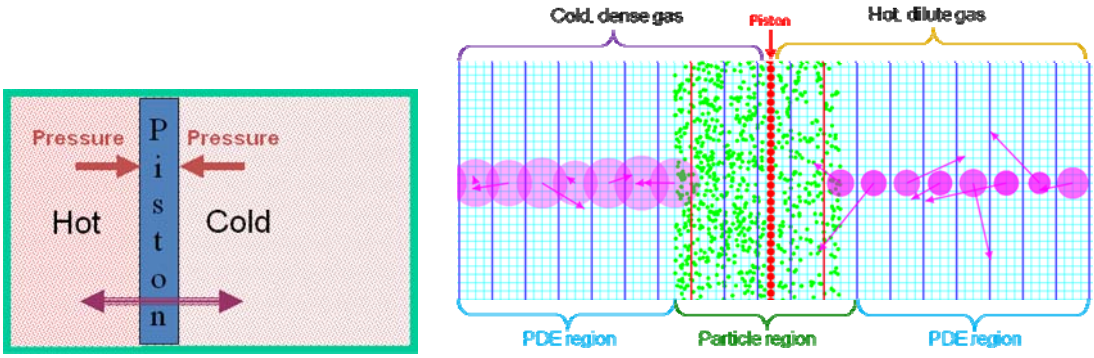

Figure 3: Adiabatic Piston problem. Schematic (left); AR hybrid snap-shot (right).

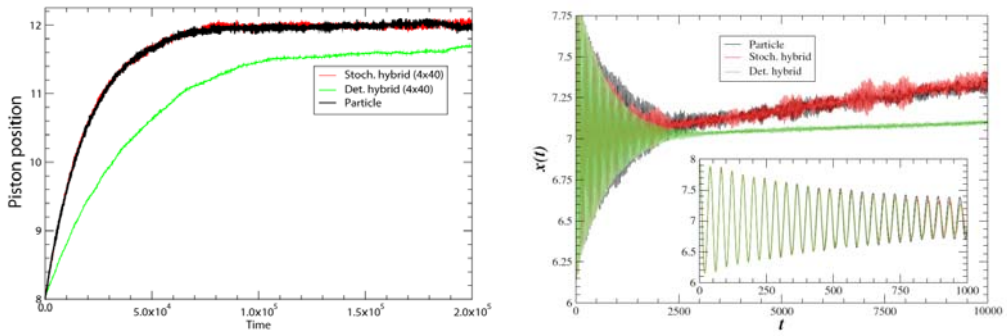

Figure 4: Time-relaxation of the position of the adiabatic piston in AR hybrid simulations. Initial mechanical equilibrium (left); initial mechanical non-equilibrium (right).

5.0 NON-IDEAL GASES

5.1 Equation of State in DSMC

In DSMC the various collision models allow for realistic representations of internal degrees of freedom, which yield accurate heat capacities, and of transport properties, such as the viscosity and thermal conductivity. However, the equation of state in standard DSMC is always that of an ideal gas, $P = N\,k\,T/V$. Fundamentally, pressure is the rate at which momentum is transferred perpendicular to a unit surface and for an ideal gas this transfer is entirely due to the ballistic motion of the particles. In DSMC there is also the collisional transfer of momentum when particles within a cell execute a collision. As discussed in Section 2, this collisional transfer introduces an error in the viscosity. Interestingly, the pressure is unaffected because of a symmetry in the selection of collision partners, specifically, particles moving towards each other are as likely to collide as those moving apart. Since the relative velocity is uncorrelated

with the relative position the virial, $\Delta \boldsymbol{v}_{ij} \cdot \boldsymbol{r}_{ij}$, is zero on average and thus the collisional contribution to the pressure is zero.

5.2 Consistent Boltzmann Algorithm

The first DSMC variant for a non-ideal gas was the Consistent Boltzmann Algorithm (CBA), which models a hard-sphere gas. [21] In CBA the collision step is modified to change the virial in order to yield the contribution to the equation of state due to the finite volume of the particles The CBA algorithm is identical to DSMC with a minor addition: After a pair of particles collides the particles are shifted by a displacement, $\boldsymbol{d}$, equal in magnitude to the hard-sphere diameter, d, and in the direction of the change of the relative velocity. That is,

$$\boldsymbol{d} = \frac{\boldsymbol{v}_{rn}' - \boldsymbol{v}_{rn}}{|\boldsymbol{v}_{rn}' - \boldsymbol{v}_{rn}|} d$$

This displacement (illustrated in Figure 5) creates a non-zero virial that correctly captures the equation of state for a dense hard-sphere gas, once the collision rate is augmented with the Enskog Y-factor (enhancement of the collision rate as a function of the volume fraction).

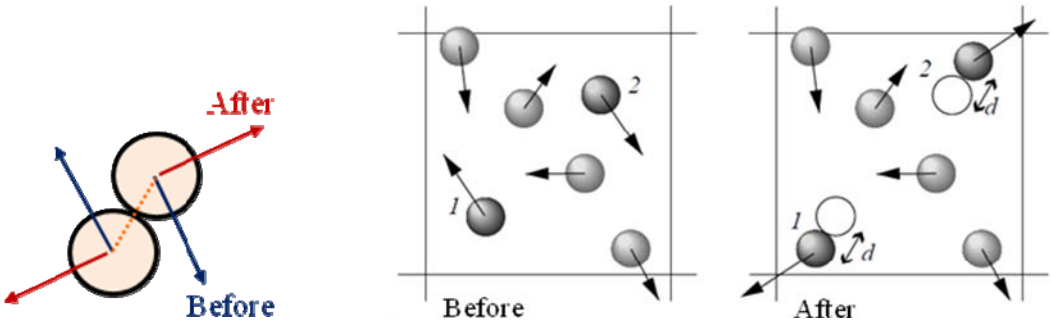

Figure 5: Correlation of relative position and relative velocity in a hard-sphere collision. (left) Displacement of particles in a CBA collision (right)

An alternative to CBA for modelling a hard-sphere gas is Enskog-DSMC in which collision partners are restricted to being a diameter apart *and* moving towards each other. [22,23] While this modification to the collision selection lowers the computational efficiency it has the advantage of having a theoretical foundation based on the Enskog equation.

5.3 Consistent Universal Boltzmann Algorithm

The CBA scheme may be generalized to model an arbitrary equation of state by making the collisional displacement a function of the local density and temperature. [24] In essence, we "reverse engineer" the displacement such that it yields the desired virial and thus the desired equation of state. This variant, called the Consistent Universal Boltzmann Algorithm (CUBA), has been demonstrated with the van der Waals equation of state and shown to capture the correct dynamics even in the condensed phase. [25] Although it is surprising that a simple variant of DSMC can model a liquid, as the density increases the computational efficiency decreases because of the increasing collision rate so CUBA is not competitive with Molecular Dynamics for the modelling of liquids. Nevertheless, for moderately dense gases it remains a useful option.

5.4 Stochastic Hard Sphere Dynamics

As discussed in the earlier sections, DSMC is being used in multi-scale simulations of Brownian motion since it is an efficient scheme for modelling the solvent. For this class of problems it is often desirable to use a dense-gas variant in order to reduce the compressibility. However, all the variants discussed above have the flaw that the variance of density fluctuations are inconsistent with the compressibility given by the equation of state. For example, in CBA the number of particles in a volume is Poisson distributed independent of the density so the density fluctuations have the same variance as for an ideal gas.

Stochastic Hard Sphere Dynamics (SHSD), another dense-gas variant for DSMC, is designed to produce the correct fluctuation spectrum consistent with the equation of state. [26] The collision process for SHSD is illustrated in Figure 6. Particles move ballistically between collisions, as in standard DSMC. When two particles, i and j, are less than a diameter apart ($|\boldsymbol{r}_{ij}| < d$) there is a probability rate ($3\chi/d$) v_n for them to collide, where $v_n = -\boldsymbol{v}_{ij} \cdot \boldsymbol{r}_{ij}/|\boldsymbol{r}_{ij}|$; particles only collide if they are approaching (i.e., if $v_n > 0$). If the collision is accepted then it is evaluated *deterministically* as if the particles had a hard-sphere diameter of $d_s = |\boldsymbol{r}_{ij}|$. The SHSD model has dynamics equivalent to a fluid with a linear core pair potential. [27]

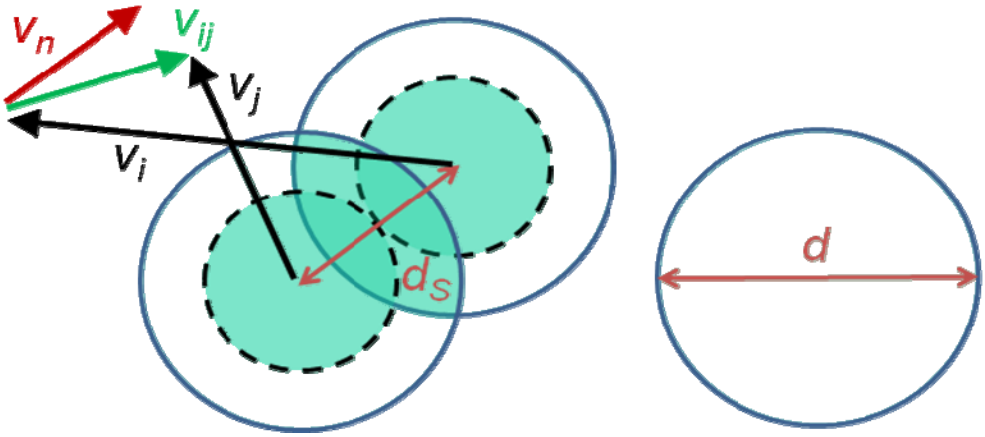

Figure 6: Schematic illustration of a Stochastic Hard Sphere Dynamics (SHSD) collision

6.0 CONCLUDING REMARKS

Direct Simulation Monte Carlo is for the computational scientist what the Boltzmann equation is to the mathematical theorist. The popularity of DSMC over the past 50 years has been, in large part, to its intuitive simplicity. Readers who have never used the method are strongly encouraged to set aside an afternoon and write a simple DSMC program to calculate viscosity (the author's textbook [3] describes this exercise in greater detail). Once the program is completed (and debugged!) it will produce the Chapman-Enskog result to good accuracy in about ten minutes. When you contrast this with the tedious mathematical calculation required using the Boltzmann equation you will appreciate the power and utility of DSMC.

7.0 REFERENCES

[1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Clarendon, Oxford (1994).

[2] M.P. Allen and D.J. Tildesley, *Computer Simulation of Liquids*, Clarendon, Oxford (1987).

[3] A. Garcia, *Numerical Methods for Physics*, Benjamin Cummings, San Francisco (2000).

[4] M. Matsumoto and T. Nishimura, *ACM Transactions on Modeling and Computer Simulation* **8** 3 (1998).

[5] A. Garcia and B. Alder, *Journal of Computational Physics*, **140** 66 (1998).

[6] A. Garcia and W. Wagner, *Journal of Computational Physics*, **217** 693 (2006).

[7] D.J. Rader, M.A. Gallis, J.R. Torczynski, and W. Wagner, *Physics of Fluids*, **18** 077102 (2006).

[8] F. Alexander, A. Garcia, and B. Alder, *Physics of Fluids,* **10** 1540 (1998).

[9] N. Hadjiconstantinou, *Physics of Fluids,* **12** 2634 (2000).

[10] M. A. Gallis, J. R. Torczynski, D. J. Rader, and G. A., Bird, *Journal of Computational Physics*, **228** 4532 (2009).

[11] D. Bruno, M. Capitelli, S. Longo, P. Minelli, *Chemical Physics Letters*, **422**, 571 (2006).

[12] M. Malek Mansour, A. Garcia, G. Lie and E. Clementi, *Physical Review Letters,* **58** 874 (1987).

[13] N. Hadjiconstantinou, A. Garcia, M. Bazant, and G. He, *Journal of Computational Physics,* **187** 274-297 (2003).

[14] Al-Mohssen, H.A., Hadjiconstantinou, N.G., *Mathematical Modeling and Numerical Analysis*, **44**, 1069-1083, (2010).

[15] G.A. Radtke, N.G. Hadjiconstantinou, and W. Wagner, *Physics of Fluids*, 23, 030606, (2011).

[16] D.C. Wadsworth and D.A. Erwin, *AIAA Paper* 90:1690 (1990).

[17] A. Garcia, J. Bell, Wm. Y. Crutchfield and B. Alder, *Journal of Computational Physics,* 154 134-55 (1999).

[18] J.B. Bell, A. Garcia, and S. Williams, *Physical Review E* **76** 016708 (2007).

[19] A. Donev, E. Vanden-Eijnden, A. Garcia, and J. B. Bell, *Communications in Applied Mathematics and Computer Science*, **5** 149 (2010).

[20] A. Donev, J.B. Bell, A. Garcia, and B. Alder, *SIAM Multiscale Modeling and. Simulation,* **8** 871-911 (2010).

[21] F. Alexander, A. Garcia and B. Alder, *Physical Review Letters,* **74** 5212 (1995).

[22] A. Frezzotti, *Physics of Fluids,* **9** 1329 (1997).

[23] J. M. Montanero and A. Santos, *Physics of Fluids,* **9** 2057 (1997).

[24] F. Alexander, A. Garcia and B. Alder, *Physica A* **240** 196 (1997).

[25] N. Hadjiconstantinou, A. Garcia, and B. Alder, *Physica A* **281** 337-47 (2000).

[26] A. Donev, B.J. Alder, and A. Garcia, *Physical Review Letters*, **101** 075902 (2008).

[27] A. Donev, B.J. Alder, and A. Garcia, *Journal of Statistical Mechanics*, P11008 (2009).